

UNCLASSIFIED

---

AD 296 970

*Reproduced  
by the*

ARMED SERVICES TECHNICAL INFORMATION AGENCY  
ARLINGTON HALL STATION  
ARLINGTON 12, VIRGINIA



---

UNCLASSIFIED

NOTICE: When government or other drawings, specifications or other data are used for any purpose other than in connection with a definitely related government procurement operation, the U. S. Government thereby incurs no responsibility, nor any obligation whatsoever; and the fact that the Government may have formulated, furnished, or in any way supplied the said drawings, specifications, or other data is not to be regarded by implication or otherwise as in any manner licensing the holder or any other person or corporation, or conveying any rights or permission to manufacture, use or sell any patented invention that may in any way be related thereto.

CATALOGED BY ASIA

AS AD No. 296970

296970

296 970

TECHNICAL NOTE

EIGENVALUES OF FERMION DENSITY MATRICES

by

Fukashi Sasaki

Quantum Chemistry Group  
For Research in Atomic, Molecular and Solid-State Theory  
Uppsala University, Uppsala, Sweden

May 1, 1962

The research reported in this document  
has been sponsored in part by the  
AERONAUTICAL RESEARCH LABORATORY, OAR,  
THROUGH THE EUROPEAN OFFICE, AEROSPACE RESEARCH,  
UNITED STATES AIR FORCE.

TECHNICAL NOTE

EIGENVALUES OF FERMION DENSITY MATRICES

by

Fukashi Sasaki<sup>\*</sup>

Quantum Chemistry Group  
For Research in Atomic, Molecular and Solid-State Theory  
Uppsala University, Uppsala, Sweden

\* This work was performed while the author  
was on leave from the Department of  
Physics, University of Tokyo, Tokyo, Japan

May 1, 1962

The research reported in this document  
has been sponsored in part by the  
AERONAUTICAL RESEARCH LABORATORY, OAR,  
THROUGH THE EUROPEAN OFFICE, AEROSPACE RESEARCH,  
UNITED STATES AIR FORCE.

## ABSTRACT

The least upper bound of the eigenvalues of second order density matrices for a system of fermions is proved to be  $n$  for a system of  $2n$  or  $2n+1$  identical fermions. It is also shown that this limiting state may be interpreted as a system of  $n$  identical pairs behaving as quasi-bosons.

## 1. INTRODUCTION

It is known that some features of a system are illustrated by the spectrum of its first-order density matrix. For example, an eigenvalue of this matrix may be interpreted as the occupation number of the corresponding spin-orbital, and if all the eigenvalues are equal to 1, the state can be described by a single Slater determinant <sup>1)</sup>. We might expect that the spectrum of a higher-order density matrix would also characterize the structure of the system. However, it seems that little has been done along this line <sup>2)</sup>. In this paper, we discuss the range of the eigenvalues of a many-particle density matrix in order to approach this problem.

---

1) Per-Olov Löwdin, Phys. Rev. 97, 1474 (1955)

2) See, however, the preliminary report of A.J. Coleman, Canad. Math. Bull. 4, No. 2, May (1961). Further progress has been reported by him at Sanibel Island, Winter Institute in Quantum Chemistry and Solid State Physics, January 2-13, 1961.

---

For this purpose, it is convenient to use a wave function expanded in terms of the eigenfunctions of density matrices <sup>3)</sup>. The expansion is obtained

---

3) B.C. Carlson and J.M. Keller, Phys. Rev. 121, 659 (1961)

---

by the use of the following theorems.

Theorem 1. If  $A$  is a linear operator which renders a completely continuous transformation <sup>4)</sup> of one Hilbert space into another, and  $f$  is an element of the first Hilbert space,  $Af$  can be written in the form

$$Af = \sum_i \mu_i g_i (f_i f).$$

---

4) See e.g. F. Riesz and B. Sz Nagy, Functional Analysis, (Frederick Ungar Publishing Company, New York 1955) pp 206

---

Here  $\{f_i\}$  and  $\{g_i\}$  are orthonormal sets in the two Hilbert spaces involved, and  $\{\mu_i\}$  is a non-increasing sequence of positive numbers. The sequence can be finite or infinite, and in the latter case it tends to zero.

Corollary 1:

$$\sup |(Af, g)| / \sqrt{(f, f)(g, g)} = \mu_1.$$

Theorem 2. If there exists a normal operator  $S$  such that  $AS = A$ , every  $f_i$  is an eigenelement of  $S$ , i.e.  $Sf_i = f_i$ .

Although special cases of Theorem 1 have been proven by others<sup>3, 5)</sup>, it would be useful to present it in a more general form. The proof of the above theorems is given in the Appendix A.

---

5) A.T. Amos and G.G. Hall, Proc. Roy. Soc. A263, 483 (1961).

---

A normalized wave function  $\Psi(x_1, x_2, \dots, x_N)$  of  $N$  fermions may be regarded as a kernel of the operator  $A$ , which transforms absolute square integrable functions of  $M$  fermions into those of  $N - M$  fermions:

$$g(x_1, \dots, x_{N-M}) = \int \dots \int dx'_1 \dots dx'_M \Psi(x_1, \dots, x_{N-M}, x'_1, \dots, x'_M) f(x'_1, \dots, x'_M),$$

or, in a brief form

$$g(x) = \int \Psi(x, y) f(y) dy,$$

where  $x$  and  $y$  denote  $(x_1 \dots x_{N-M})$  and  $(x'_1 \dots x'_M)$  respectively. Since the wave function  $\Psi(x, y)$  is normalized:

$$\iint |\Psi(x, y)|^2 dx dy = 1,$$

it renders necessarily a completely continuous transformation (for a proof, see the Appendix B). By the use of Theorem 1, we obtain the following expansion of the wave function  $\Psi$ :

$$\Psi(x, y) = \sum_i \mu_i g_i(x) f_i(y), \quad (1-1)$$

where

$$\int g_i^*(x) g_j(x) dx = \delta_{ij},$$

$$\int f_i^*(y) f_j(y) dy = \delta_{ij}$$

and

$$\mu_i \geq \mu_j > 0 \quad \text{for} \quad i < j.$$

Since the density matrix of order  $M$  of this pure state is defined by

$$\Gamma_M(y, y') = \binom{N}{M} \int \Psi(x, y) \Psi^*(x, y') dx$$

we obtain immediately the diagonal expansion of the density matrix from (1-1) in the form

$$\Gamma_M(y, y') = \binom{N}{M} \sum_i \mu_i^2 f_i(y) f_i^*(y').$$

Similarly the density matrix of order  $N-M$  is found to be

$$\Gamma_{N-M}(x, x') = \binom{N}{M} \sum_i \mu_i^2 g_i(x) g_i^*(x').$$

In order to evaluate the symmetry property of  $f_i$ , it is convenient to introduce the antisymmetry projection operator defined with respect to the coordinates  $y = (x_1' \dots x_M')$ :

$$O_{AS, y} = \frac{1}{M!} \sum_P \epsilon_P P.$$

Here  $P$  is a permutation operator which permutes only the coordinates  $y$  and  $\epsilon_P$  is its parity. It is easy to see that  $O_{AS, y}$  is self-adjoint and that

$$\int \Psi(x, y) O_{AS, y} f(y) dy = \int O_{AS, y} \Psi(x, y) f(y) dy = \int \Psi(x, y) f(y) dy.$$

Thus by using Theorem 2, it follows that  $O_{AS, y} f = f$ , i.e. that if the function  $\Psi$  is antisymmetric,  $f_i$  and  $g_i$  in the expansion (1-1) should also be antisymmetric.



## 2. THE LEAST UPPER BOUND

The largest eigenvalue of a density matrix of order  $M$  may be regarded as a functional of  $\Psi$ :

$$\lambda_{M,N}(\Psi) = \binom{N}{M} \mu_1^2.$$

Introducing a projection operator  $O_\Psi$  which projects out the state  $\Psi$ :

$$O_\Psi = \Psi \Psi^\dagger,$$

we obtain the following equality from (1-1);

$$\lambda_{M,N}(\Psi) = \binom{N}{M} (g, f, O_\Psi g, f).$$

Introducing the total antisymmetry projection operator

$$O_{AS} = \frac{1}{N!} \sum_P \varepsilon_P P,$$

it is found for any function  $\omega = \omega(x, y)$  that

$$\begin{aligned} (\omega (O_{AS} - O_\Psi) \omega) &= (\omega (1 - O_\Psi) O_{AS} (1 - O_\Psi) \omega) = \\ &= ((1 - O_\Psi) \omega O_{AS} (1 - O_\Psi) \omega) \geq 0. \end{aligned}$$

Thus we obtain the following inequality

$$\begin{aligned} \lambda_{M,N}(\Psi) &\leq \binom{N}{M} (g, f, O_{AS} g, f) \leq \\ &\leq \binom{N}{M} \sup_{f,g} (g f O_{AS} g f), \end{aligned} \quad (2-1)$$

where  $f$  and  $g$  are normalized functions of  $M$  and  $N-M$  particles, respectively. Since the last term of (2-1) does not depend on  $\Psi$ , it follows that

$$\lambda_{M,N} \equiv \sup_{\Psi} \lambda_{M,N}(\Psi) \leq \binom{N}{M} \sup_{f,g} (g f O_{AS} g f). \quad (2-2)$$

We shall now prove that the last term of (2-2) is equal to  $\lambda_{M,N}$ . Let  $\{f^{(k)}\}$  and  $\{g^{(k)}\}$  be the sets of normalized functions which give a

solution of the above extremum problem:

$$0 < \lambda^{(k)} \equiv \binom{N}{M} (g^{(k)} f^{(k)} O_{AS} g^{(k)} f^{(k)}) \rightarrow \binom{N}{M} \sup_{f, g} (g f O_{AS} g f)$$

as  $k \rightarrow \infty$ .

Since a set of functions  $\{\Psi^{(k)}\}$  defined by the equation

$$\Psi^{(k)} = \sqrt{\binom{N}{M} / \lambda^{(k)}} O_{AS} g^{(k)} f^{(k)}$$

consists of normalized antisymmetric functions, it follows from Corollary 1 that

$$\lambda_{M, N}(\Psi^{(k)}) \geq \binom{N}{M} |(g^{(k)} f^{(k)}, \Psi^{(k)})|^2 = \lambda^{(k)},$$

i.e. that

$$\lim_{k \rightarrow \infty} \lambda_{M, N}(\Psi^{(k)}) \geq \lim_{k \rightarrow \infty} \lambda^{(k)} \quad (2-3)$$

By comparing (2-3) with (2-2), it is found that

$$\lambda_{M, N} = \binom{N}{M} \sup_{f, g} (g f O_{AS} g f)^{6)} \quad (2-4)$$

6)

We note that for a system of identical bosons, the whole argument is valid by replacing the antisymmetry projection operators by the symmetry projection operators. Thus the least upper bound of the eigenvalues for bosons is given by the equation

$$\lambda_{M, N} = \binom{N}{M} \sup_{f, g} (g f O_S g f) \quad (2-5)$$

under the condition  $(f, f) = (g, g) = 1$ . Here the total symmetry projection operator  $O_S$  is given by the equation

$$O_S = \frac{1}{N!} \sum_P P$$

It is readily seen from (2-5) that

$$\lambda_{M, N} = \binom{N}{M}. \quad (\text{for a system of bosons})$$

### 3. UPPER BOUNDS

It is convenient to write the antisymmetry projection operator in the form

$$\binom{N}{M} O_{AS}(1, \dots, N) = O_{AS}(1, \dots, M) O_{AS}(M+1, \dots, N) \times$$

$$\sum_{i=0}^{\min\{N-M, M\}} (-1)^i \binom{N-M}{i} \binom{M}{i} P\{(1, M+1)(2, M+2) \dots (i, M+i)\} O_{AS}(1, \dots, M) O_{AS}(M+1, \dots, N) \quad (3-1)$$

where  $O_{AS}(p \dots g)$  denotes the antisymmetry projection operator defined with respect to the coordinates in the parenthesis, and  $P\{(1, M+1)(2, M+2) \dots (i, M+i)\}$  denotes the operation of replacing the coordinate 1 by  $M+1$ ,  $M+1$  by 1, ...,  $i$  by  $M+i$  and  $M+i$  by  $i$ . This shows that  $f$  and  $g$  which give the extremum in the equation (2-4) should be antisymmetric. Therefore we may introduce the density matrices of the  $i$ -th order  $\Gamma_{i,f}$  and  $\Gamma_{i,g}$  reduced from  $f$  and  $g$ . By the use of these density matrices, we obtain

$$\lambda_{M,N} = 1 + \sup \sum_{i=1}^{\min(M, N-M)} (-1)^i \text{tr } \Gamma_{i,f} \Gamma_{i,g}. \quad (3-2)$$

Since density matrices are positive definite, it is easy to see that

$$0 \leq \text{tr } \Gamma_{i,f} \Gamma_{i,g} \leq \min(\text{tr } \Gamma_{i,f} \lambda_{i, N-M}; \text{tr } \Gamma_{i,g} \lambda_{i, M}) =$$

$$= \min \left[ \binom{M}{i} \lambda_{i, N-M}; \binom{N-M}{i} \lambda_{i, M} \right]. \quad (3-3)$$

From (3-2) and (3-3) we obtain an upper bound of the eigenvalues by the recurrence equation

$$\lambda_{M,N} \leq \Lambda_{M,N} = 1 + \sum_{i=1}^{\min\left\{\left[\frac{M}{2}\right], \left[\frac{N-M}{2}\right]\right\}} \min \left[ \binom{M}{2i} \Lambda_{2i, N-M}; \binom{N-M}{2i} \Lambda_{2i, M} \right]. \quad (3-4)$$

The solutions of (3-4) are

---

7)  $[x]$  stands for the integral part of  $x$ .

$$\begin{aligned}
 \Lambda_{0,N} &= 1 \\
 \Lambda_{1,N} &= 1 \\
 \Lambda_{2,N} &= \left[ \frac{N}{2} \right] & N \geq 6 \\
 \Lambda_{3,N} &= 1 + 3 \left[ \frac{N-3}{2} \right] & N \geq 6 \\
 \Lambda_{4,N} &= 1 + \left( \left[ \frac{N}{4} \right] - 1 \right) \left( 1 + 6 \left[ \frac{N}{2} \right] - 6 \left[ \frac{N}{4} \right] \right) + (N - 4 \left[ \frac{N}{4} \right]) (N - 4 \left[ \frac{N}{4} \right] - 1) \\
 & & N \geq 8 \\
 \Lambda_{5,N} &= 1 + 10 \left[ \frac{N-5}{2} \right] + 5 \Lambda_{4,N-5} & N \geq 10 \\
 &\vdots
 \end{aligned}$$

It should be noticed that

$$\Lambda_{M,N} = O(N^{\lfloor \frac{M}{2} \rfloor}).$$

This is the same order of magnitude as the largest eigenvalue of  $\Gamma_{\lfloor \frac{M}{2} \rfloor}$  for a system of  $\lfloor \frac{N}{2} \rfloor$  bosons.

Since the eigenvalues of the first order density matrix of a single determinant wave function are 1,  $\Lambda_{1,N}$  is equal to  $\lambda_{1,N}$ . It is shown in Section 5 that  $\Lambda_{2,N}$  is also equal to  $\lambda_{2,N}$ .

#### 4. EXTREME PROPERTIES OF WAVE FUNCTIONS

In this section we study the case where the largest eigenvalue of the  $M$ -th order density matrix is almost equal to the least upper bound  $\lambda_{M,N}$ . Suppose we have a wave function  $\Psi$  such that

$$(f, \Gamma_{M,N} f) = \lambda_{M,N} - \epsilon$$

where  $\epsilon$  is a small non-negative number and  $f$  is a normalized function of  $M$  particles. It should be noted that  $f$  may or may not be an eigenfunction of  $\Gamma_{M,N}$ . Define a function  $\Phi$  by the equation

$$\Phi(1, \dots, N) = \sqrt{\binom{N}{M} / \lambda_{M,N}} O_{AS} f(1, \dots, M) g(M+1, \dots, N)$$

where

$$g_{(M+1, \dots, N)} = \sqrt{\binom{N}{M} / (\lambda_{M,N} - \epsilon)} \int \dots \int \Psi(1, \dots, N) f^*(1, \dots, M) dx_1 \dots dx_M.$$

It is easy to see that

$$(g, g) = \frac{1}{\lambda_{M,N} - \epsilon} (f \Gamma_{M,\Psi} f) = 1,$$

$$\begin{aligned} (\Psi, \Phi) &= \sqrt{\binom{N}{M} / \lambda_{M,N}} (\Psi \circ_{As} f g) = \\ &= \sqrt{\binom{N}{M} / \lambda_{M,N}} (\Psi, f g) = \\ &= \sqrt{1 - \frac{\epsilon}{\lambda_{M,N}}} \end{aligned}$$

and

$$(\Phi, \Phi) = \binom{N}{M} (f g \circ_{As} f g) / \lambda_{M,N} \leq 1$$

Then it follows that

$$\begin{aligned} 0 &\leq (\Psi - \Phi, \Psi - \Phi) = (\Psi, \Psi) + (\Phi, \Phi) - (\Psi, \Phi) - (\Phi, \Psi) \leq \\ &\leq 2 - 2 \sqrt{1 - \frac{\epsilon}{\lambda_{M,N}}} \leq \frac{2 \epsilon}{\lambda_{M,N}} \end{aligned} \quad (4-1)$$

From the first three terms of (4-1), we obtain

$$(\Phi, \Phi) \geq 2 \sqrt{1 - \frac{\epsilon}{\lambda_{M,N}}} - 1 \geq 1 - \frac{2 \epsilon}{\lambda_{M,N}}$$

Summarizing the results obtained above, we have a theorem.

**Theorem 3.** If a normalized M-particle function  $f$  satisfies the following equation

$$(f | \Gamma_{M, \Psi} | f) = \lambda_{M, N} - \epsilon,$$

the wave function  $\Psi$  can be expressed as

$$\Psi = \sqrt{\binom{N}{M} / \lambda_{M, N}} O_{AS} f(1, \dots, M) g_{(M+1, \dots, N)} + h(1, \dots, N),$$

where  $(g, g) = 1$ ,  $(h, h) \leq \frac{2\epsilon}{\lambda_{M, N}}$  and  $1 \geq (\Psi | h, \Psi | h) \geq 1 - \frac{2\epsilon}{\lambda_{M, N}}$ .

We apply the above theorem to the first order density matrix. We know that some of the eigenvalues of the first order density matrix can be  $\lambda_{1, N(=1)}$ ,

$$\Gamma_{1, \Psi}(1, 1') = \sum_{i=1}^p f_i(1) f_i^*(1') + \sum_{i=p+1} \lambda_i f_i(1) f_i^*(1').$$

In such a case, it follows from Theorem 3 that the wave function  $\Psi$  can be expressed as

$$\Psi = \sqrt{N} O_{AS} f_1(1) g_1(2, \dots, N) \quad (4-3)$$

Using (3-1), we obtain

$$1 = (\Psi, \Psi) = N (f_1 | g_1 | O_{AS} f_1 | g_1) = 1 - \int \dots \int dx_2 \dots dx_{N-1} | \int f_1^*(1) g_1(1, 2, \dots, N-1) dx_1 |^2$$

i.e.

$$\int dx_1 f_1^*(1) g_1(1, 2, \dots, N-1) = 0. \quad (4-4)$$

The first order density matrix of  $g$  is found from (4-3) and (4-4) to be

$$\Gamma_{1, g_1} = \Gamma_{1, \Psi} - \Gamma_{1, f_1}. \quad (4-5)$$

Comparing (4-2) with (4-5), we see that the largest eigenvalue of  $\Gamma_{1, g_1}$  is also 1 if  $p > 1$ . Thus by repeated application of the previous discussion, it

is found that

$$\Psi = \sqrt{\frac{N!}{(N-p)!}} O_{AS} f_1(1) \dots f_p(p) g(p+1, \dots, N), \quad (4-6)$$

$$\Gamma_{1, \Psi} = \sum_{i=1}^p f_i x f_i + \Gamma_{1, g} \quad (4-7)$$

and

$$\int dx_i f_i^*(1) g(1, 2, \dots, N-p) = 0 \quad (4-8)$$

(i = 1, \dots, p)

## 5. THE LEAST UPPER BOUND OF THE EIGENVALUES OF THE SECOND ORDER DENSITY MATRICES

In this section, we prove that the upper bound  $\Lambda_{2, N}$  derived in Section 3 is actually the smallest.

Define functions  $F_{2n}(1 \dots 2n)$  and  $F_{2n+1}(1 \dots 2n+1)$  by the equations

$$\begin{aligned} F_{2n}(1, \dots, 2n) &= O_{AS} f(1, 2) f(3, 4) \dots f(2n-1, 2n) \\ F_{2n+1}(1, \dots, 2n+1) &= O_{AS} f(1, 2) f(3, 4) \dots f(2n-1, 2n) g(2n+1) \end{aligned} \quad (5-1)$$

where  $f(1, 2)$  is a normalized antisymmetric function of two particles and  $g(1)$  is an arbitrary normalized function of a particle.

Then it is found that

$$(F_{2n}, F_{2n}) = \frac{2^n n!}{(2n)!} + O(\epsilon^2) \quad (5-2)$$

$$(F_{2n+1}, F_{2n+1}) = \frac{2^n n!}{(2n+1)!} + O(\epsilon) \quad (5-2')$$

where

$$\varepsilon^2 = \text{tr} (\Gamma_1, f)^2 = \iiint f(1,2) f(3,4) f^*(1,3) f^*(2,4) dx_1 dx_2 dx_3 dx_4. \quad (5-3)$$

Proof

$$\begin{aligned} (F_{2n}, F_{2n}) &= (O_{AS} f \cdots f, O_{AS} f \cdots f) = \\ &= (f \cdots f O_{AS} f \cdots f) = \\ &= \frac{1}{(2n)!} \sum_P \varepsilon_P (f \cdots f P f \cdots f) \\ &= \frac{1}{(2n)!} \sum_P a_P, \end{aligned}$$

where  $a_P = \varepsilon_P (f \cdots f P f \cdots f)$ . There exist  $2^n n!$  permutations which interchange the particles keeping every pair. It is easy to see that  $a_P = 1$  for such a permutation since  $\varepsilon_P P f \cdots f = f \cdots f$ , but otherwise  $a_P$  is the order of  $\text{tr}(\Gamma_{1,f})^2$ .

For odd  $N$ , (5-2') can be similarly proven. In this case some of the permutations will give integrals of the order  $\text{tr}(\Gamma_{1,f} \Gamma_{1,g})$ , but

$$0 \leq \text{tr} \Gamma_{1,f} \Gamma_{1,g} \leq \sqrt{\text{tr} (\Gamma_{1,f})^2 \text{tr} (\Gamma_{1,g})^2} = \sqrt{\text{tr} (\Gamma_{1,f})^2} = \varepsilon.$$

Q.E.D.

$$\text{Let } \Psi^N(1, \dots, N) = F_N(1, \dots, N) / \sqrt{(F_N, F_N)}. \quad (5-4)$$

Using (3-1), (5-2) and (5-2') we obtain

$$\begin{aligned} (\Psi^N, \Psi^N) &= 1 = \\ &= \frac{(F_{N-2}, F_{N-2})}{(F_N, F_N)} (f \Psi^{N-2} O_{AS} f \Psi^{N-2}) = \\ &= \frac{1 - \text{tr} \Gamma_{1,f} \Gamma_{1,\Psi^{N-2}} + (f \Gamma_{2,\Psi^{N-2}} f)}{\left[ \frac{N}{2} \right] + O(\varepsilon)}. \end{aligned}$$



Here we have used a trivial equality

$$O_{AS}(1, \dots, N) = O_{AS}(3, \dots, N) O_{AS}(1, \dots, N) O_{AS}(3, \dots, N).$$

Since  $\text{tr } \Gamma_{1,f} \Gamma_{1,\Psi^{N-2}} = O(\epsilon)$ , we finally obtain

$$(\int \Gamma_{2,\Psi^N} f) = \left[ \frac{N}{2} \right] + O(\epsilon). \quad (5-5)$$

It is possible to make  $\text{tr}(\Gamma_{1,f})^2$  as small as we wish, and therefore the largest eigenvalue of  $\Gamma_{2,\Psi^N}$  can be arbitrarily close to  $\Lambda_{2,N}$ .

It is found further that a wave function  $\Psi$  can be approximated by the form (5-4), if the largest eigenvalue is close to  $\Lambda_{2,N}$ . To prove this, suppose we have an N-particle wave function  $\Psi$  and a 2-particle function  $f$  such that

$$(\int \Gamma_{2,\Psi} f) = \left[ \frac{N}{2} \right] + \epsilon \quad (5-6)$$

Then using Theorem 3 and (3-1), we obtain

$$\Psi = \sqrt{\binom{N}{2} / \Lambda_{2,N}} O_{AS} f g_1 + h_1$$

where  $(h_1 | h_1) < 2\epsilon / \Lambda_{2,N}$ ,

and

$$\begin{aligned} 1 - \frac{2\epsilon}{\Lambda_{2,N}} &\leq \binom{N}{2} (\int g_1 O_{AS} f g_1) / \Lambda_{2,N} = \\ &= \{1 - \text{tr } \Gamma_{1,f} \Gamma_{1,g_1} + (\int \Gamma_{2,g_1} f)\} / \Lambda_{2,N}. \end{aligned}$$

Since  $\text{tr } \Gamma_{1,f} \Gamma_{1,g} > 0$ , we see that

$$(\int \Gamma_{2,g_1} f) \geq \Lambda_{2,N-2} - 2\epsilon \quad (5-7)$$

showing that the function  $g_1$  can be again expressed as

$$g_1 = \sqrt{\binom{N-2}{2} / \Lambda_{2,N-2}} O_{AS} f g_2 + h_2$$

where  $(h_2|h_2) < 4\epsilon/\Lambda_{2,N-2}$ . Repeating the procedure, we obtain a decomposition of the total wave function  $\Psi$ :

$$\begin{aligned}\Psi &= \sqrt{\binom{N}{2}}/\Lambda_{2,N} O_{AS} f[\sqrt{\binom{N-2}{2}}/\Lambda_{2,N-2} O_{AS} f[\{\dots\}] + h_2] + h_1 \\ &= \frac{N!}{2^{\frac{N}{2}} (N/2)!} O_{AS} f(1,2) f(3,4) \dots f(N-1,N) + h(1,\dots,N) \quad (N: \text{even}) \\ &= \frac{N!}{2^{\frac{N-1}{2}} (\frac{N-1}{2})!} O_{AS} f(1,2) f(3,4) \dots f(N-2,N-1) g(N) + h(1,\dots,N) \quad (N: \text{odd})\end{aligned}$$

where  $(h|h) = O(\epsilon)$ .

Q.E.D.

By using (5-3), the first order density matrix can be written in the form

$$\begin{aligned}\Gamma_{1,\Psi} &\simeq \frac{N}{2} \Gamma_{1,f} \quad (N: \text{even}) \\ &\hspace{15em} (5-9) \\ \Gamma_{1,\Psi} &\simeq \frac{N-1}{2} \Gamma_{1,f} + g)(g. \quad (N: \text{odd})\end{aligned}$$

The expressions (5-8) and (5-9) suggest that such a state may be interpreted as a system of fermion pairs which occupy the same state. These electron pairs behave like quasi-bosons and, since they are all in the same state, the limiting wave function corresponds to a situation with complete Bose-Einstein condensation.

#### ACKNOWLEDGEMENT

The author is indebted to Professor P.O. Löwdin, Professor A.J. Coleman and Dr. L.B. Rédei for helpful discussions and criticism. To Professor Löwdin, the author would like to express his gratitude for giving him the opportunity of being in the stimulating atmosphere of the Quantum Chemistry Group.

# APPENDIX A

Let  $f$  and  $g$  be elements of two Hilbert spaces  $E$  and  $E'$  respectively, and  $A$  be a linear operator which is completely continuous and hence transforms every infinite and bounded set in  $E$  into a compact set in  $E'$ . If  $A$  is not a zero operator, there exists a sequence  $\{f^{(n)}\}$  such that

$$\|f^{(n)}\| = 1 \quad \text{and} \quad \|Af^{(n)}\| \rightarrow \sup_{f \in E} \|Af\|/\|f\| = \mu_1$$

where  $\mu_1 > 0$ . From the compactness of  $\{Af^{(n)}\}$ , it follows that the sequence  $\{Af^{(n)}/\mu_1\} \equiv \{g^{(n)}\}$  contains a subsequence  $\{g^{(n_k)}\}$  which converges to an element  $g_1$  of  $E'$ . The norm of  $g_1$  is 1, since  $\|g^{(n_k)}\| = \frac{1}{\mu_1} \|Af^{(n_k)}\| \rightarrow 1$ .

In addition, the sequence  $\{f^{(n_k)}\}$  itself converges to an element  $f_1$  of  $E$ . Consider a linear functional  $K(f) = (Af, g_1)$ . The least upper bound of  $|K(f)| \equiv \nu$  on the sphere  $\|f\| = 1$  is equal to  $\mu_1$ . To prove  $\nu \geq \mu_1$ , consider the sequence  $\{f^{(n_k)}\}$ . Then

$$\nu \geq |K(f^{(n_k)})| = |(Af^{(n_k)}, g_1)| \rightarrow \mu_1 \quad (k \rightarrow \infty).$$

On the other hand

$$\begin{aligned} \nu &= \lim_{m \rightarrow \infty} |(Af^{(m)}, g_1)| = \frac{1}{\mu_1} \lim_{m \rightarrow \infty} \lim_{k \rightarrow \infty} |(Af^{(m)}, Af^{(n_k)})| \leq \\ &\leq \frac{1}{\mu_1} \overline{\lim_{m \rightarrow \infty}} \|Af^{(m)}\| \lim_{k \rightarrow \infty} \|Af^{(n_k)}\| \leq \mu_1 \end{aligned}$$

where  $\{f^{(m)}\}$  is a sequence which gives

$$|K(f^{(m)})| \rightarrow \nu \quad \text{as} \quad m \rightarrow \infty.$$

Thus we obtain

$$\begin{aligned} \|f^{(n_k)} - f^{(n_l)}\|^2 &= 4 - \|f^{(n_k)} + f^{(n_l)}\|^2 \leq \\ &\leq 4 - \frac{|K(f^{(n_k)} + f^{(n_l)})|^2}{\mu_1^2} = 4 - \frac{|K(f^{(n_k)}) + K(f^{(n_l)})|^2}{\mu_1^2} \\ &\rightarrow 4 - \frac{|\mu_1 + \mu_1|^2}{\mu_1^2} = 0, \end{aligned}$$

since  $|K(f)| < \mu_1 \|f\|$  for any  $f \in E$ . Thus we can conclude that  $f^{(n_k)}$  converges to an element  $f_1$  of  $E$  as a result of the completeness of  $E$ .

It is easy to see that the elements  $f_1$  and  $g_1$  satisfy the equation

$$A f_1 = g_1 \mu_1$$

$$\text{since } A f^{(n_k)} = \mu_1 g^{(n_k)} \quad \text{for any } n_k.$$

We note that

$$\sup_{\substack{f \in E \\ g \in E'}} |(A f, g)| = \mu_1$$

under the condition  $\|f\| = \|g\| = 1$ , since

$$\mu_1 = (A f_1, g_1) \leq \sup |(A f, g)| \leq \sup \|A f\| \cdot \|g\| = \mu_1.$$

Repeating the above procedure in the subspace of  $E$  which consists of all the elements orthogonal to  $f_1$ , we obtain a pair of elements ( $f_2$  and  $g_2$ ), and  $\mu_2$ , if  $A$  is not a zero operator in the subspace. In general,  $f_k$  and  $g_k$  are obtained as a solution of the following extremum problem;

$$(A f_k, g_k) = \sup_f \|A f\| / \|f\| = \mu_k > 0 \quad (A-1)$$

under the conditions  $\|f_k\| = \|g_k\| = 1$  and  $(f_i, f) = 0$  ( $i = 1, 2, \dots, k-1$ ). This procedure terminates when  $\mu_k$  vanishes. It follows that

$$A f_k = \mu_k g_k$$

and moreover that the set  $\{g_k\}$  is an orthonormal set. This follows from the evaluation

$$\begin{aligned} \|\alpha g_k + \beta g_l\|^2 &= |\alpha|^2 + |\beta|^2 + 2 \Re(\bar{\alpha} \beta (g_k, g_l)) = \\ &= \|A(\frac{\alpha}{\mu_k} f_k + \frac{\beta}{\mu_l} f_l)\|^2 \leq \\ &\leq \mu_k^2 \|\frac{\alpha}{\mu_k} f_k + \frac{\beta}{\mu_l} f_l\|^2 = |\alpha|^2 + \frac{\mu_k^2}{\mu_l^2} |\beta|^2 \\ &\quad (k < l). \end{aligned}$$

Setting  $\beta = \alpha(g_l, g_k) \frac{\mu_l^2}{\mu_k}$  we obtain

$$|(g_k, g_l)|^2 \left(1 + \frac{\mu_l^2}{\mu_k^2}\right) \leq 0.$$

Hence  $(g_k, g_l) = 0$ .

The sequence  $\{\mu_n\}$  is evidently composed of monotonically decreasing and positive terms

$$\mu_1 \geq \mu_2 \geq \dots > 0.$$

We can prove that  $\mu_k \rightarrow 0$  as  $k \rightarrow \infty$  if the sequence is infinite. If  $\mu_k \rightarrow \mu > 0$ , the sequence  $\{\mu_k g_k\} = A\{f_k\}$ , which is a bounded sequence  $\{f_k\}$  transformed by  $A$ , would not contain a convergent subsequence, since

$$\|\mu_k g_k - \mu_l g_l\|^2 = \mu_k^2 + \mu_l^2 \geq 2\mu^2 > 0 \quad \text{for } k \neq l.$$

An arbitrary element of  $E$  may be expressed as

$$f = \sum_{i=1}^n (f_i, f) f_i + f^{(n)}, \quad (\text{A2})$$

where  $f^{(n)}$  is orthogonal to  $f_i$  ( $i = 1, 2, \dots, n$ ) and

$$\|f^{(n)}\|^2 = \|f - \sum_{i=1}^n (f_i, f) f_i\|^2 = \|f\|^2 - \sum_{i=1}^n |(f_i, f)|^2 \leq \|f\|^2.$$

Therefore if the sequence  $\{\mu_i\}$  is infinite,

$$\|A f^{(n)}\| \leq \mu_{n+1} \|f^{(n)}\| \leq \mu_{n+1} \|f\| \rightarrow 0$$

as  $n \rightarrow \infty$ . Operating by  $A$  on both sides of (A-2) and taking the limit, we obtain

$$A f = \sum_{i=1}^{\infty} (f_i, f) A f_i = \sum_{i=1}^{\infty} \mu_i (f_i, f) g_i.$$

In the case where the sequence  $\{\mu_i\}$  terminates at  $\mu_k$ , it follows from (A-1) that

$$\|A f^{(k)}\| = 0.$$

Thus we obtain

$$A f = \sum_{i=1}^k \mu_i (f_i, f) g_i$$

This proves Theorem 1.

It follows from Theorem 1 that

$$\begin{aligned} (A f, g) &= \sum_i \mu_i (f, f_i) (g_i, g) \leq \sqrt{\sum_i \mu_i^2} \|f\| \sqrt{\sum_j | (g_j, g) |^2} \leq \\ &\leq \mu_1 \|f\| \|g\| \end{aligned}$$

Setting  $f = f_1$  and  $g = g_1$ , we obtain

$$(A f_1, g_1) = \mu_1$$

Thus, we have proven Corollary 1.

To prove Theorem 2, let  $S$  be a normal operator such that

$$A S = A .$$

Then

$$\begin{aligned} \|(1-S)f_i\|^2 &= ((1-S)(1-S^*) f_i, f_i) = ((1-S)(1-S^*) f_i, f_i) = \\ &= \frac{1}{\mu_i} (A (1-S)(1-S^*) f_i, g_i) = \frac{1}{\mu_i} (0, g_i) = 0. \end{aligned}$$

This proves Theorem 2.

## APPENDIX B

In order to prove that the transformation under consideration is completely continuous, we shall show that any weakly convergent sequence  $\{f_n(y)\}$  is transformed by  $\Psi(x, y)$  into a strongly convergent sequence  $\{g_n(x)\}$ .

From (1-1) it follows that the function

$$k(x) = \int |\Psi(x, y)|^2 dy$$

has a definite and finite value for almost all  $x$ . Therefore, since  $\{f_n(y)\}$  is weakly convergent,

$$g_n(x) - g_m(x) = \int \Psi(x, y) f_n(y) dy - \int \Psi(x, y) f_m(y) dy$$

tends to 0 almost everywhere when  $m, n \rightarrow \infty$ .

Using Schwarz's inequality, we have

$$\begin{aligned} |g_n(x)|^2 &= \left| \int \Psi(x, y) f_n(y) dy \right|^2 \leq \int |\Psi(x, y)|^2 dy \int |f_n(y)|^2 dy \leq M k(x) \\ &\leq \int |\Psi(x, y)|^2 dy \int |f_n(y)|^2 dy \leq M k(x) \end{aligned}$$

Here a finite number  $M$  is an upper bound of a sequence  $\{\int |f_n(y)|^2 dy\}$ .

Then

$$|g_n(x) - g_m(x)|^2 \leq |g_n(x)|^2 + |g_m(x)|^2 + 2|g_n(x)g_m(x)| \leq 4Mk(x)$$

Since  $4Mk(x)$  is a Lebesgue-integrable function and we have shown that

$|g_n(x) - g_m(x)|^2$  tends to 0 almost everywhere, it follows from Lebesgue's theorem that

$$\int |g_n(x) - g_m(x)|^2 dx \rightarrow 0$$

when  $n, m \rightarrow \infty$ .

Q. E. D.

Uppsala University, Sweden Quantum Chemistry Dept Rep. No. AD	Contract AF 61(052)-351 TN 77	Uppsala University, Sweden Quantum Chemistry Dept Rep. No. AD	Contract: AF 61(052)-351 TN 77
Monitoring Agency: USAF, EOOAR	FIELD: Physics	Monitoring Agency: USAF, EOOAR	FIELD: Physics
EIGENVALUES OF FERMION DENSITY MATRICES.		EIGENVALUES OF FERMION DENSITY MATRICES.	
Fukashi Sasaki	May 1, 1962	Fukashi Sasaki	May 1, 1962
ABSTRACT: The least upper bound of the eigenvalues of second order density matrices is proved to be $n$ for a system of $2n$ or $2n+1$ identical fermions. It is also shown that this limiting state may be interpreted as a system of $n$ identical pairs.		ABSTRACT: The least upper bound of the eigenvalues of second order density matrices is proved to be $n$ for a system of $2n$ or $2n+1$ identical fermions. It is also shown that this limiting state may be interpreted as a system of $n$ identical pairs.	
USAF, European Office, OAR, Brussels, Belgium		USAF, European Office, OAR, Brussels, Belgium	
Uppsala University, Sweden Quantum Chemistry Dept Rep. No. AD	Contract AF 61(052)-351 TN 77	Uppsala University, Sweden Quantum Chemistry Dept Rep. No. AD	Contract: AF 61(052)-351 TN 77
Monitoring Agency: USAF, EOOAR	FIELD: Physics	Monitoring Agency: USAF, EOOAR	FIELD: Physics
EIGENVALUES OF FERMION DENSITY MATRICES.		EIGENVALUES OF FERMION DENSITY MATRICES.	
Fukashi Sasaki	May 1, 1962	Fukashi Sasaki	May 1, 1962
ABSTRACT: The least upper bound of the eigenvalues of second order density matrices is proved to be $n$ for a system of $2n$ or $2n+1$ identical fermions. It is also shown that this limiting state may be interpreted as a system of $n$ identical pairs.		ABSTRACT: The least upper bound of the eigenvalues of second order density matrices is proved to be $n$ for a system of $2n$ or $2n+1$ identical fermions. It is also shown that this limiting state may be interpreted as a system of $n$ identical pairs.	
USAF, European Office, OAR, Brussels, Belgium		USAF, European Office, OAR, Brussels, Belgium	